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Global Tropospheric Experiment: Chemical Instrumentation Test and Evaluation-3 (GTE/CITE3) -Mission Scientist Program-

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Final Report

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A. Program Objectives

The success and experience gained from CITE-1 and 2 provided the framework for designing the CITE-3 mission. The specific mission objectives of the CITE-3 mission as related to sulfur in the troposphere were:

(1) To test and evaluate via airborne field intercomparisons the capability to make reliable measurements of the concentrations of the following sulfur species: sulfur dioxide (SO_2), dimethylsulfide (DMS), carbonyl sulfide (COS), carbon disulfide (CS_2), and hydrogen sulfide (H_2S).

(2) To determine in a predominantly marine environment (coastal zones included) the abundance and distribution of major sulfur species over a wide range of atmospheric conditions, including altitude, solar flux levels, atmospheric mixing, and surface source strengths of sulfur.

The first of these objectives represented a continuation of the GTE/CITE philosophy with the emphasis on sulfur rather than the nitrogen species. The second objective, as in CITE-2, reflects the recognition that instrument intercomparison and atmospheric science need not be mutually exclusive. In particular, the CITE-2, mission demonstrated that well-defined science issues can be addressed during an instrument evaluation mission. However, in CITE-3, as in CITE-2, instrument intercomparison was considered the primary focus of

the program and, indeed, only by achieving this objective was it possible to address the science objectives.

B. Completed Project Tasks

(1) Field Mission

Starting from August 17 and running through September 27, 1989, the mission scientist played a major role in planning and directing a total of 19 CITE-3 missions on NASA's Lockheed Electra. The first ten missions were flown from NASA's Wallops Flight Facility (WFF); two involved the transit from Wallops, Virginia to Natal, Brazil via an overnight stop in Barbados; and seven missions were flown while operating out of Natal, brazil. In each case, the flights were predominantly, if not entirely, over a marine environment. From an inspection of the sulfur concentration ranges reported during the field operation as well as from a more critical analysis of the data post mission, it is quite evident that a robust data set was generated for purposes of carrying out the proposed sulfur intercomparison study.

The scientific portion of CITE-3 was predominantly focused on the WFF → Natal transit flight plus the seven missions based out of Natal. The major emphasis of these flights was that of examining the vertical and horizontal distributions and levels of the sulfur species DMS, SO_2, and COS. In addition, considerable time was devoted to examining the diurnal trends in the levels of DMS under known meteoro-

logical conditions. The results, as viewed in the field and in post mission analysis showed a very significant diurnal trend for this sulfur species, thus making possible DMS flux calculations. It also appears that in virtually all cases the conditions under which the flights were carried out were such that the source of SO_2 in the marine B.L. was predominantly that of B.L. oxidation of surface emitted DMS.

As a final comment on field mission activities, it is to be noted that the mission scientist was successful in organizing a group of scientist to help collect and subsequently analyze nearly 70 hydrocarbon samples as part of the CITE-3 non-sulfur support measurement program.

(2) Data Analysis/Data Review Workshop

This investigator worked closely with Jim Hoell and Gerry Gregory, (including having advanced meetings at Langley), to review the statistical analysis to be used in examining the CITE-3 sulfur data base. This involved a detailed examination of all analyses that Dr. Gregory had carried out up through April of 1990.

During the data workshop, in addition to reviewing all CITE-3 data, the mission scientist took this opportunity to explore with CITE-3 investigators the possibility of coordinating their efforts for the upcoming AGU meeting as well as coordinating their efforts on all future JGR manuscript submissions. It was agreed upon, in fact, that

there would be only one major science paper written for each sulfur species, i.e. SO_2, CS_2, COS, H_2S, & DMS. This decision did not preclude any number of instrument papers being written as related to measurement techniques for each of the sulfur species. The mission scientist was also able to get agreement on the preparation of several non-sulfur related science papers, e.g. nitrogen budget, test of photochemical theory, and O_3 photochemical tendency.

The results from the data workshop on CITE-3, suggested that measurements of DMS, CS_2, H_2S, and COS could be carried out with some confidence using current techniques.

The results for SO_2 were far more problematic. There clearly is some evidence that suggest that at least one of the techniques may be very reliable as an SO_2 field instrument; however, since there were no two instruments that were in good agreement throughout the intercomparison period, the latter conclusion is based primarily on correlations with the other ancillary data collected during the flights. It would appear, therefore, that further intercomparisons work will be necessary on SO_2 measurement techniques.

(3) AGU Presentations and Sulfur Workshop

The first release of CITE-3 data to the public domain was scheduled during the Fall 1990 AGU meeting in San Francisco. The mission scientist played a major role at this meeting, giving two presentations and being a co-author on three

others, see list below:

AGU meeting San Francisco Dec. 1990

(1) Operational Overview of NASA GTE/CITE-3 Airborne Expt., D.D. Davis, J.M. Hoell, G. Gregory, and R. Bendura.

(2) Airborne Sulfur Trace Species Intercomparison Campaign: Sulfur Dioxide, Dimethylsulfide, Hydrogen Sulfide, Carbon Disulfide, and Carbonyl Sulfide, G.L. Gregory, J.M. Hoell, and D.D. Davis.

(3) Atmospheric Non-Methane Hydrocarbon Measurements on the NASA/GTE/CITE-3 Mission, M.O. Rodgers, D.D. Davis, J.E. Martinez, S. Smyth, J.D. Bradshaw, J. Schendel, P. Zimmerman, J.B. Greenberg, and D. Blake.

(4) Photostationary State Implications of CITE-3 NO_2/NO Measurements, J.D. Bradshaw, G. Chen, D.D. Davis, S.T. Sandholm, G.L. Greogory, J.D. Barrick, and G. Sachse.

(5) O_3 Photochemical Tendency in the Tropical South Atlantic as Determined From the NASA CITE-3 Mission: D.D. Davis, W.L. Chameides, J.D. Bradshaw, S.T. Sandholm, J. Schendel, G. Sachse, G. Gregory, and B. Anderson.

(4) Modelling

The immediate short term goal of the mission scientist was that of developing a versatile photochemical box model (i.e. a model that could be installed and operated on a portable PC) that could be used in the field in a real-time

evaluation mode. The longer term goal was to use the output from the model (based on the finalized CITE-3 data base) to provide a more comprehensive interpretation of the CITE-3 sulfur data base. In particular, OH and H_2O_2 concentration levels are needed for purposes of understanding the diurnal trends in DMS and to explain the altitudinal gradients in both DMS and SO_2.

During the active time period of this grant (Jan. 1989 - Jan. 1991), a "Clean-Air" photochemical box model was successfully developed which proved to be very versatile in terms of being fully compatible with a portable PC having 1 MB of main memory and at least 10 MB of hard drive disk space. Nevertheless, following the CITE-3 field mission, it was found that the hydrocarbon samples collected during the mission contained very substantial levels of C_2 - C_9 hydrocarbons. This is now believed to have resulted from a combination of long range transport of biomass emissions from Africa and local pollution caused by large ships moving from Europe to Brazil. Based on these new hydrocarbon data, test runs on the "Clean Air" model indicated that OH levels would be substantially influenced and that the only reliable means of modelling the lower and middle troposphere would be to build a photochemical box model that contained full non-methane hydrocarbon chemistry. Subsequently, an evaluation was carried out of the three major hydrocarbon models being used in the modelling community and the decision was to use the

"CAL" model as modified to include full isoprene chemistry. The inclusion of the "CAL" hydrocarbon chemistry is now complete. Thus at this time, the on-going Photochemical Box Model is capable of handling all known chemistries for tropospheric environments ranging from regions nominally labelled "polluted" to regions that are "pristine". As noted below, new modelling results are now forthcoming as related to predicted OH, HO_2, and H_2O_2 levels, species that have the greatest impact on sulfur chemistry.

C. Future Activity

The major future activity as related to the CITE-3 mission will involve the writing and publication of results. The latter effort will necessarily involve further modelling efforts, in particular, the development of a "time-dependent" component for the already operational box model. The latter should be completed by the end of the summer 1991.

It is expected that the continued analysis of the CITE-3 data base will lead to the publications listed below. In each case, this author has indicated the level of contribution he is expecting to make to bring each paper to a final state of completion. It should be noted that I am proposing that the completion of all CITE-3 data analysis and all writing and publishing of CITE-3 results be financed by a new NASA grant now being submitted by D. Davis and W. Chameides, i.e. "Diagnostic Studies of the H_xO_y-N_xO_y-O_3-Halogen-Sulfur

Photochemical System Using Data from NASA GTE Field Operations."

Publications In-Preparation as Related to CITE-3

Intercomparison of CITE-3 CS_2 Measurements	Co-author
Intercomparison of CITE-3 H_2S Measurements	Co-author
Intercomparison of CITE-3 DMS Measurements	Co-author
Intercomparison of CITE-3 COS Measurements	Co-author
Intercomparison of CITE-3 SO_2 Measurements	Co-author
DMS Diurnal Trends and Estimates of Ocean Fluxes in the Tropical South Atlantic	Major co-author
SO_2 vertical gradients in the Tropical South Atlantic as Observed During NASA's CITE-3 Mission	Major co-author
O_3 Photochemical Tendency in the North and South Tropical Atlantic as Observed During NASA's CITE-3 Mission	Lead author
An Operational Overview of the NASA CITE-3 Program	Major co-author
A Test of NO_2/NO Photochemical Theory Based on Results from NASA's CITE-3 Mission	Lead author